SIMULATIONS OF SELF-ORGANIZATION AND DEFECT REPAIR IN ORGANIC SURFACES THAT INTERACT WITH BIOMOLECULES

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Abstract
Self-assembled monolayers-SAMs-represent an ideal model system for studying the role of defect mechanisms, self-organization and repair on the adhesion of biological macromolecules. SAMs are attractive for use in such diverse biological applications as selective protein binding, controlled cell growth and death, protein resistance, and fabrication (patterning) because they are easily formed and are very stable at room temperature. The SAMs most studied are short functionalized alkane thiols (HS-(CH2)n-R) where the S atoms chemically bond to a Au (111) surface and the terminal R groups collectively form a layer exposed to solution. The terminal group of the thiol, R, can be funtionalized in wide variety of ways that dramatically change the chemistry, and therefore properties, of the surface. These terminal groups can, for example, render the SAM protein resistant or absorbing. We have recently carried out extensive molecular dynamics simulations on defect and defect-free ethylene glycol terminated SAMs (HS-(CH2)11-(O CH2CH2)6-OH; Chin and Whitesides unpublished) on Au in an effort to study the ability of these systems to resist or promote the adsorption of proteins. Our simulations suggest that the conformation of the thiols, and the structure of the waters proximate to the surface of the SAM are very different between the two systems, and provide a hypothesis that the cohesive energy within the SAM and the binding of interfacial waters are two important indicators of the properties of these SAMs. These simulations are therefore useful in understanding-and ultimately designing-surfaces that resist non-specific binding (important in emerging microanalytical technologies), that promote cell growth and death, and that provide fundamental insights into binding with biologically relevant molecules. In other words, providing new insight into organic surfaces useful for the study of cancerous cells, and for the development of micro and nano sensors.